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# Grid-Free Electrostatic Particle Simulations

**Introduction** This report summarizes work done between September 2007 and June 2008 related to the development of a set of grid-free simulation tools for problems in plasma dynamics. As noted in the abstract on page one, the research objectives are: (1) to develop a grid-free field solver, fluid model, and kinetic model, (2) to evaluate these tools in comparison with traditional mesh-based methods, and (3) to demonstrate the capability of the grid-free approach in an application of USAF interest.

The past year's work has focused on: (1) Grid-free 3D Direct Simulation Monte Carlo and optimal parallel implementation, (2) application of grid-free Direct Simulation Monte Carlo methods to the continuous wave formation of a Bose Einstein condensate and Hypersonic Flows and, (3) Validation of grid-free agents MONICO and G2. (4) Boundary integral methods and Regularized Particles, (5) Boundary Integral Corrected PIC-An Advanced Subcell Method (6) Extended the treecode to kernels of the form  $re^{-cr}$ , ideal for spacecraft plume simulations. The work accomplished has provided several key results, as described below.

Basic plasma science plays an increasingly significant role in applications of importance to the United States Air Force (USAF). These include the study of satellites and how they interact with an ion engine, the use of electronic tethers to protect satellites and how solar eruptions effect satellites. Additional examples include the basic physics of magnetrons for use in directed energy (DE) systems, the prediction and prevention of arc formation in DE systems, understanding intense laser-plasma interaction as it relates to space propulsion, "non-destructive" materials testing for turbine blades in aircraft, and the study of Penning traps as a potential way of trapping anti-protons and positrons to create and store anti-hydrogen as a fuel, etc.

The above plasma applications are examples of plasmas which require a fully kinetic description in at least part of the domain. The most common approach to simulating these types of systems is to make use of a fully Lagrangian framework, where the model is reduced to tracking the evolution of test particles in phase space. Of the many varieties, the most accepted approach is Particle-In-Cell (PIC) [1]. The PI, with his collaborators, is developing an alternative approach, the Boundary Integral Treecode (BIT) [2] and Gridless DSMC. BIT is based on fast summation algorithms, which eliminates the need for a fixed volumetric mesh. Gridless DSMC uses the clustering strategy of BIT to determine collision partners and combines this with mesh free interpolation to track flow averages [3,4].

In a range of numerical experiments, the all scale resolution of BIT has proven to provide a substantial improvement over traditional PIC [2]. Further, the Gridless DSMC has demonstrated the ability to more accurately capture flow fields for nonuniform flow fields, such as in hyper sonic flows [3,4]. The Parallel version of the Gridless DSMC has been tested for scalability and is currently scaling at about 90 percent up-to 128 nodes of a distributed memory machine, and it has

not been test beyond this. Further, the gridless DSMC appears to avoid issues of cell interface temperature jumps due to the stochastic nature of the tree clustering algorithm. The randomness can be attributed to the fact that the clustering is combined with Monte Carlo collisions which adds randomness to particle properties.

The BIT method has been shown to have significantly less numerical heating than explicit PIC codes [5]. The objective in this currant work is to develop a grid-free electromagnetic formulation of BIT. BIT is a numerical Green's function method based on discretization of the integral formulation of the problem. In the electromagnetic case, the Green's function is time dependent and therefore discretization in time requires that a time history be maintained. The issue of a time history has already been addressed for time dependent Green's functions with stationary point sources [7,8]. However, for moving point sources, the time history is still a computational issue, since every step introduces  $N$  new sources which need to be maintained for all future time. One approach to handle this issue is the to use a coarse fixed underlying mesh for tracking the effect of distant moving charges.

As a first step towards the electromagnetic case, we are exploring the use of a coarse fixed mesh for domain decomposition in electrostatic problems, where BIT is used as a sub-cell method within each PIC cell [6]. The methods presented here differ from Particle-Particle-Particle-Mesh (P3M) in that local boundary integrals are used within each cell to provide an accurate description of the local fields within a mesh cell [9]. We demonstrate that, in 1D, regularized BIT corrected PIC substantially reduces numerical heating, even when  $\Delta x \gg \lambda_D$ . We expect that  $\Delta x \gg \lambda_D$  should increase the efficiency of large scale PIC calculations, enhancing the capability of legacy PIC codes by adding both fidelity (less numerical heating) and efficiency (allowing more flexibility in meshing at a given level of fidelity). For a wide class of electromagnetic problems, where PIC is used, this electrostatic work is beneficial, since for stability, the mesh spacing is sufficiently small that the system looks electrostatic. In collaboration with AFRL/DEHE, the PI is working on incorporating this into ICEPIC. This work is intended to complement our planned study of the use of fast summation methods in compressing the time history for time depended moving sources.

**New Efforts (Sep 2007 to Present):** PI Karsny and PI Christlieb have been working on the extinction of the integral methods to mesh based systems for the ease of coupling grid-free solvers with grid based solvers and we are working on three papers. PI Karsny has put substantial effort into the development of recurrence relations for kernels of the form  $re^{-cr}$  so that they may be incorporated into the adaptive treecode framework, which he is in the process of writing this up. This is critical for the modeling of neutral as well as dense plasmas simulations. While we heave not included this work here, it will stand as a key pice of a white paper we will be submitting in the near future. PI Christlieb has focused on the impact of regularization on solutions in BIT and BIT corrected PIC through analysis, development of high order  $C^\infty$  'localized' regularization and how it improves the solution in BIT and BIT corrected PIC, development of truly localized high order ( $C^n$ ) regularization in BIT (PI and Dr. Ong), the devilment and analysis of high order correction inside spectral deferred correction (SDC) (PI and Dr. Qiu), definition of a new metric (accuracy criterion) for a fair comparison between single step methods and deferred correction methods (PI,

Dr. Ong and Dr. Qiu), the application 12 order SDC to BIT simulations of one and two stream instability (PI, Dr. Ong and Dr. Qiu) and the application of high order SDC to BIT simulations with point-insertion (PI and Dr. Ong). Objective of the work with Dr. Ong and Dr. Qiu is to develop a truly high order particle method. Since efforts with Dr. Ong and Dr. Qiu are now just coming into there own, the PI will details these in the 2008 spring review, August 13-15, for computational math. Additional work with Dr. Cartwright has focused on high order time stepping in PIC and the possibility of truly implementing an efficient high order method in the ICEPIC framework. This is only computationally effect because of the information that is already stored for the parallel framework and the thought s that this method may not be particularly efficient in a serial PIC code. Efforts to make the particle push not have a self force is the primary focus of this effort. The PI has been collaborating with Dr. Cartwright on this effort for about nine months. Finely, the PI and Dr. Olson (a former student) are pursuing the application of Gridless DSMC to hypersonic flows, orbital station keeping and and plume modeling of trusters. We are working with Dr. Ong on combining the 3D gridless DSMC with 3D BIT so at to provide accurate mesh free simulations of arc formation. On another note, I am please to inform AFOSR that my former student, Dr. Olson will be joining AFRL Kirtland DEHE as a full time research scientist. Dr. Cartwright, Dr. Olson, Dr. Ong and the PI are starting to discuss a four way collaboration on arc and spark formation in wave guides.

**Below is a brief outline of BIT corrected PIC. Deities of the work can be found in an attached paper which was just submitted for publication. The Gridless DSMC has been accepted for publication. Again, a brief review is below. Details can be found in the attached preprint. I have also include a biographical sketch, detailing recent accomplishments.**

**Electrostatic BIT** Given a collection of  $N$  macro-particles interacting through a long range coulomb force, the question becomes what is the most efficient way to evaluate the self fields for a desired accuracy. For a collection of charged particles in a bounded domain the electrostatic potential is given by the solution of,

$$\nabla^2 \phi(\mathbf{x}) = -1 \frac{\rho(\mathbf{x})}{\epsilon_o}, \quad \rho(x) = \sum_{j=1}^N q_j \delta(\mathbf{x} - \mathbf{x}_j), \quad \{\mathbf{x}, \mathbf{x}_j\} \in \Omega / \partial\Omega \quad (1)$$

where  $\phi$  is the electrostatic potential,  $\epsilon_o$  is the permittivity of free space,  $\rho(\mathbf{x})$  is the charge density,  $\{q_j, \mathbf{x}_j\}$  is the charge/location on a given test particle,  $\Omega$  is the domain and  $\partial\Omega$  is the boundary of  $\Omega$ . The problem may have Dirlet, Neumann, mixed or periodic boundary conditions along  $\partial\Omega$ .

In general, the solution to equation (1) for any right hand side may be expressed as,

$$\phi(\mathbf{x}) = -1 \left( \int_{\Omega} \frac{\rho(\mathbf{y})}{\epsilon_o} G(\mathbf{x}|\mathbf{y}) d\mathbf{y} + \oint_{\partial\Omega} \phi(\mathbf{y}) \partial_{n_y} G(\mathbf{x}|\mathbf{y}) + G(\mathbf{x}|\mathbf{y}) (\partial_{n_y} \phi(\mathbf{y})) ds \right) \quad (2)$$

where we chosen  $G$  to be the free space Green's function,  $\phi(\mathbf{y})$  and  $(-\partial_{n_y} \phi(\mathbf{y}))$  are the potential and normal electric field along  $\partial\Omega$ . The problem would be over determined if both  $\phi(\mathbf{y})$  and  $(-\partial_{n_y} \phi(\mathbf{y}))$  were specified at each point  $\mathbf{y} \in \partial\Omega$ . The unknown function is determined by imposing consistence,

$$\lim_{\mathbf{x} \rightarrow \mathbf{y}} \phi(\mathbf{x}) = \phi(\mathbf{y}) \quad or \quad \lim_{\mathbf{x} \rightarrow \mathbf{y}} \partial_{n_x} \phi(\mathbf{x}) = \partial_{n_y} \phi(\mathbf{y}) \quad (3)$$

wherever  $\phi(\mathbf{y})$  or  $(\partial_{n_y}\phi(\mathbf{y}))$  is specified along  $\partial\Omega$ .

The integral equation for the unknown function,  $\gamma$  or  $\sigma$ , is solved using numerical quadrature and the resulting matrix is inverted using a modified GMRES [2]. The resulting system looks like a collection of  $N$  particles. The electric field at particle  $i$  is given by,

$$\mathbf{E}(\mathbf{x}_i) = \sum_{j=1, j \neq i}^N \frac{q_j}{\epsilon_0} \nabla_{\mathbf{x}} G(\mathbf{x}|\mathbf{x}_j)|_{\mathbf{x}=\mathbf{x}_i} - \nabla_{\mathbf{x}} B.C. |_{\mathbf{x}=\mathbf{x}_i} \quad (4)$$

where  $B.C.$  stands for boundary correction term. The primary issue with equation (4) is that the order of operations count is  $O(N^2)$ . In most simulations,  $N$  may range from several hundred thousand to tens of millions of test particles, which makes the calculation prohibitively expensive.

To overcome the  $O(N^2)$  issue, BIT makes use of a fast summation algorithm. There are many variants of fast summation algorithms, in this case we are making use of the Treecode algorithm. The idea is to approximate the long range interaction of each distant cluster of particles as a moment expansions about the center of each cluster. Since plasma problems are dynamic, the algorithm constructs the clusters using bisection algorithm recursively in space, this creates a hierarchical tree sorting of the particles. Fields are computed using a recursive divide and conquer approach, which makes use of the tree for determining the appropriate approximations in computing the long range interactions [2]. The method is  $O(N \log N)$ , a substantial speedup over direct summation. (Note that PIC is  $O(M \log M)$  where  $M$  is the number of mesh elements.)

**BIT Corrected PIC** Our goal is to provide legacy PIC codes with a robust and accurate sub-cell method for field calculations, minimizing numerical heating while increasing  $\Delta x \gg \lambda_D$ . The simple idea is to use regularized BIT as a sub-cell method within each PIC cell. The boundary conditions on BIT are chosen to be either the potential or field computed on a PIC mesh. The domain where BIT is applied may be chosen to be larger than a single cell. Figure 1 a) shows how the force falls off between two particles within a mesh cell (blue dashed line) and how the force behaves in 1D (solid blue line), 2D (green dashed line) and in 3D (red solid line). Figure 1 b) shows a cartoon of a PIC mesh where the red cell is the one we are considering. The domain where BIT is applied could be as small as the red cell or could be extended, as in the yellow domain, for computing the force in the red cell. In the case of the yellow domain, the boundary integral uses the PIC fields from the mesh nodes on the edge of the domain as the boundary conditions and all of the particles in the yellow domain are used in computing the field evaluations for the particles in the red domain via the treecode.

*1D Example* Consider the charge neutral test problem of  $N$  randomly placed negative test charges with a uniform background positive charge in domain  $\Omega = (a, b)$  with boundary points  $\partial\Omega = \{a, b\}$ ,

$$\frac{d^2\phi}{dx^2} = -\frac{q_0 n_0}{\epsilon_0} \left( 1 - \frac{(b-a)}{N} \sum_{i=1}^N \delta(x-x_i) \right), \quad \phi(a) = \phi(b), \quad \frac{d\phi(a)}{dx} = \frac{d\phi(b)}{dx}.$$

Let  $M$  be the number of PIC mesh cells and let the mesh spacing be  $\Delta y = (b-a)/(M-1)$ . Let the mesh points be give by  $y_i = i\Delta y + a$ ,  $i \in \{0, 1, \dots, M-1\}$ . Let  $x_j$  be the location of the test

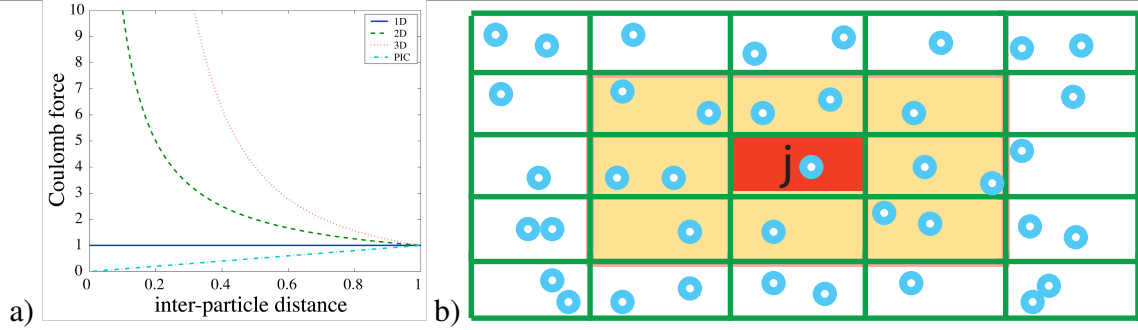


Figure 1: a) is a plot of how the fields fall off in a PIC code, as a function of distance with in the cell, as compared with the true fields. b) is a cartoon of a BIT corrected PIC mesh where the red cell is where the fields are computed with BIT on the yellow regain.

particles in  $\Omega$ . Let  $\phi_i$  be the mesh based solution to the potential at mesh cell  $i$  obtained by using an FFT (reference [1]) and let  $C_i = \{x_j | \lfloor (x_j - a)/\Delta y \rfloor = i\}$ . The sub-cell electric field using the regularized Green's function is given by,

$$\mathbf{E}^d(x_k) = \frac{q_0 n_0}{\epsilon_0} \left( x_k - \frac{(b-a)}{N} \sum_{j \in C_i, j \neq k} \frac{x_k - x_j}{\sqrt{(x_k - x_j)^2 + d^2}} \right) - \frac{1}{b-a} \left( \phi_{i+1} - \phi_i + \frac{q_0 n_0}{\epsilon_0} \left( \frac{1}{2}(b^2 - a^2) + \frac{(b-a)}{2N} \sum_{j \in C_i} \sqrt{(b-x_j)^2 + d^2} - \sqrt{(a-x_j)^2 + d^2} \right) \right). \quad (5)$$

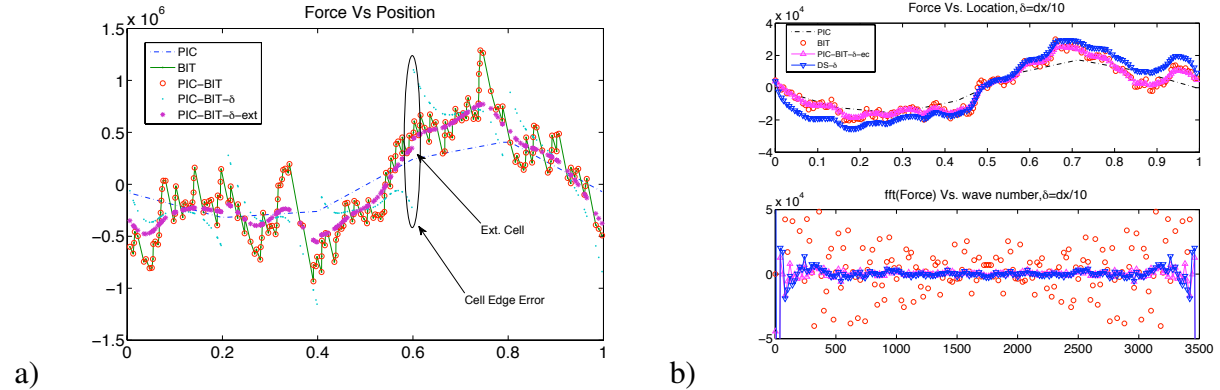


Figure 2: a) Force Vs. Location: PIC is the back dashed line, BIT is the green line with dots, BIT corrected PIC with  $d = 0$  is the open red circles, BIT corrected PIC with  $d = \Delta x/10$  is the blue dots and extend cell BIT corrected PIC is the magenta stars. b) FFT of force for three results.

Figure 2 a) shows the solution the electric field computed using PIC (the black dashed line), BIT (the green line with dots), BIT corrected PIC with no regularization (the open red circles), BIT corrected PIC with  $d = \Delta x/10$  (the blue dots) and an extended cell BIT corrected PIC with one cell on either side (magenta stars). The simulation uses 5 PIC cells and  $N = 500$  randomly placed

particles. Observe that if  $d = 0$ , BIT corrected PIC is in excellent agreement with BIT, however, if  $d$  is finite, there is divergence at the cell interfaces. The divergence at the cell interfaces is because near the boundary, the regularization pollutes the field associated with charge near the edge. The mechanism for this is well understood by the PI, the extended cell represents one possible solution. Alternatively, instead of using a regularization, one could propose a smooth limiter on the force, which would have a similar effect. Figure 2 b) shows the FFT of the force in 1D for BIT (identical to direct sum in 1D) BIT corrected PIC with extended cells and regularization and Direct Sum with regularization. Observe that the spectrum of the regularized system is much smoother.

Figure 3 shows the results for several numerical heating experiments comparing PIC, BIT and BIT corrected PIC with regularization. The system is charge neutral with 4000 electrons uniformly sampled in space and the velocity is samples from a Gaussian distribution with initial temperature  $T_e$ . The numerical integrator was Leap Frog and the runs are 100 plasma oscillations. PIC is using  $\Delta x = 16\lambda_D$  with 10 cells across the gap. The top figure in a), b) and c) shows the initial distribution (blue) and the final distributions; black-PIC, red-BIT and magenta-BIT corrected PIC with extended cells and regulation. The parameters are a)  $\Delta t = \Delta x/v_{max}/10$  and  $d = \Delta x/20$ , b)  $\Delta t = \Delta x/v_{max}/5$  and  $d = \Delta x/10$  and c)  $\Delta t = \Delta x/v_{max}/2$  and  $d = \Delta x/10$ .

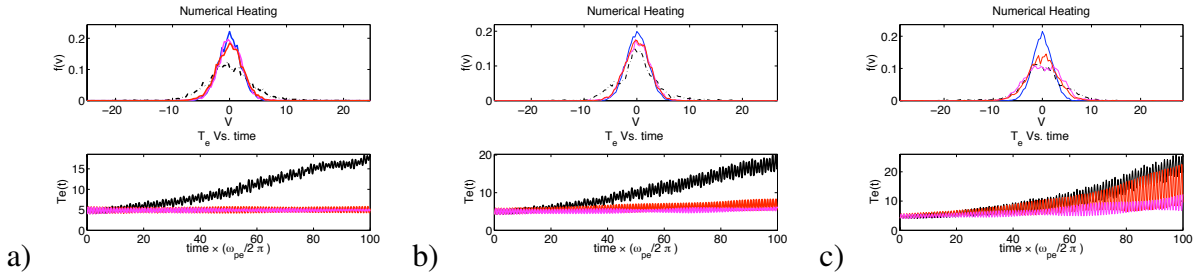


Figure 3: Numerical heating test with 4000 test particles uniformly sampled in space and sampled from a Gaussian in velocity. Black line - PIC, red line - BIT, magenta line - BIT Corrected PIC. a)  $\Delta t = \Delta x/v_{max}/10$  and  $d = \Delta x/20$ , b)  $\Delta t = \Delta x/v_{max}/5$  and  $d = \Delta x/10$  and c)  $\Delta t = \Delta x/v_{max}/2$  and  $d = \Delta x/10$

**Collisional Plasmas (Christlieb, Olson)** In order to account for collisions, the right hand side of equation (1) becomes

$$\left. \frac{\delta f}{\delta t} \right|_c = \int_{\mathbf{R}^3} \int_S (f(\mathbf{v}')f(\mathbf{v}_*) - f(\mathbf{v})f(\mathbf{v}_*)) \bar{v} \sigma d\Omega d\mathbf{v}_*,$$

where  $\bar{v}$  is the relative velocity between two particles,  $\sigma$  is the scattering cross section and  $d\Omega$  is the differential solid angle through which particles scatter. The two product terms in the parentheses represent a source and loss of particles which scatter into and out of a given velocity through collisional events. This convolution integral over velocity space is expensive to compute. One common approach to reducing the cost is to use Monte Carlo techniques.

In this work we have developed an innovative grid-free approach to Monte Carlo methods for gas dynamics problems. Again, we model  $f$  as a collection of macro particles in phase space. The evolution of the new equation (1) is carried out using operator splitting in time, i.e., we evolve the macro particles, which describe the transport of  $f$  through phase space and then correct the resulting distribution functions for collisional events using a Monte Carlo method. It has been shown that this method converges to the solution of the modified equation (1) as the particle number goes to infinity. Novel aspects in this work are that particles are clustered adaptively using octrees at each time step and that macro flow quantities are tracked and updated in the nodes of the tree using grid-free interpolation.

The method has been applied to several benchmark problems such as Couette flow, thermal Couette flow, and flow past a lifting body. In addition, we have applied the method to the study of the formation of a Bose-Einstein condensate.

*Couette and Thermal Couette* For the velocity driven Couette flow, we compared the results of our grid-free DSMC with a thoroughly tested code, MONACO.<sup>1</sup> We ran several test cases with different Knudsen numbers,  $K_n$ . The two approaches are in excellent agreement, shown in figure 4 (a) and (b). Figure 4 (a) is the temperature profile across the gap for the velocity driven Couette flow and figure 4 (b) is the velocity profile across the gap for the velocity driven flow.

Figure 4 (c) shows the results of the two methods for the temperature driven Couette flow. Again, the results of the two methods are in excellent agreement. The results for flow past a flat plate are

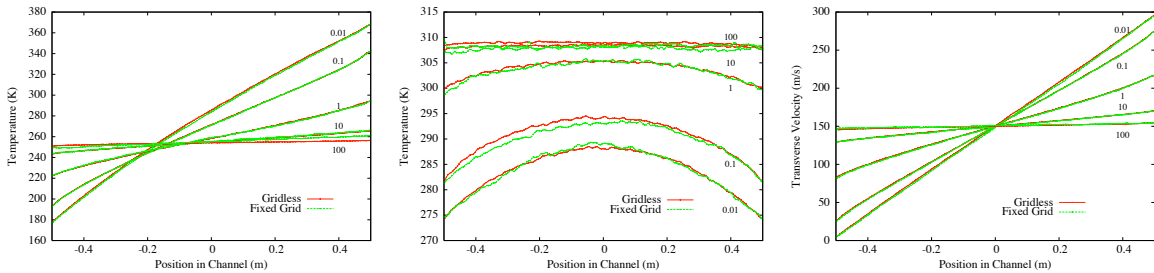


Figure 4: Simulation results for grid based and grid-free Monte Carlo simulations of thermal and velocity driven Couette flow. The images show results for a range of densities,  $k_n \in \{0.01, 0.1, 1, 10, 100\}$ . Note that  $k_n$  is the mean free path over a characteristic length, as  $k_n \rightarrow \infty$  the density goes to zero. On the far right the plot is of the temperature profile for the thermal Couette flow. The middle and left plots are the temperature and velocity profiles for the velocity driven Couette flow.

also in good agreement with previous work. Eventually this method, in combination with other grid-free tools, will be used to simulate the behavior of complex multi-species collisional plasmas in a grid-free framework. Our first papers on this method is complete and accepted to JCP (May 2008).

<sup>1</sup>Grid based DSMC Code developed by Professor Iain D. Boyd's research group, University of Michigan Aerospace



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**Personnel Supported During Duration of Grant**

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**Publications**

"Grid-Free Direct Simulation Monte Carlo," A.J. Christlieb and S. Olson, Accepted to *J. Comp. Phys.* in May 2008.

"Boundary Integral Corrected Particle-In-Cell," Andrew Christlieb and Keith Cartwright, *Submitted to SIAM J on Scientific Computing*.

"Spectral Deferred Correction Methods with High Order Runge-Kutta Schemes in Prediction and Correction steps.," Jingmei Qiu, Ben Ong and Andrew Christlieb *Submitted to AMS Mathematics of Computation*.

**Honors & Awards Received**

Air Force Young Investigator Award – awarded January 2007  
 NRC Summer Faculty Fellow – awarded March 2006

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**Transitions**

AFRL/DEHE is collaborating with the PI on transiting BIT corrected PIC into AFRL-ICEPIC.

**New Discoveries**

Numerical Heating in Particle codes can be controlled with a regularized sub-cell method (PI).

High order corrections to regularization have an important advantage near interfaces (PI).

High order corrections have an important advantage near interfaces (PI).

Analysis of oscillator problem points to why regularization is useful away from boundaries (PI and Dr. Cartwright). (Details at 08 Review)

High order correction steps inside SDC is an advantage in both efficiency and accuracy. (PI and Dr. Qiu) (Details at 08 Review)

SDC is advantage in BIT codes even when using point insertion. (PI and Dr. Ong) (Details at 08 Review)